

Adipic acid, 2-chloropropyl dodecyl ester

Inchi: InChI=1S/C21H39ClO4/c1-3-4-5-6-7-8-9-10-11-14-17-25-20(23)15-12-13-16-21(24)26-18
InchiKey: IJCBFPAXRPMNGO-UHFFFAOYSA-N
Formula: C21H39ClO4
SMILES: CCCCCCCCCCOC(=O)CCCCC(=O)OCC(C)Cl
Mol. weight [g/mol]: 390.99

Physical Properties

Property code	Value	Unit	Source
gf	-356.27	kJ/mol	Joback Method
hf	-987.39	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	84.65	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	6.181		Crippen Method
mvol	333.870	ml/mol	McGowan Method
pc	994.51	kPa	Joback Method
rinpol	2640.00		NIST Webbook
rinpol	2640.00		NIST Webbook
tb	869.45	K	Joback Method
tc	1064.76	K	Joback Method
tf	485.67	K	Joback Method
vc	1.302	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.28	J/molxK	869.45	Joback Method
cpg	1080.07	J/molxK	902.00	Joback Method
cpg	1096.68	J/molxK	934.55	Joback Method
cpg	1112.13	J/molxK	967.10	Joback Method
cpg	1126.44	J/molxK	999.66	Joback Method
cpg	1139.64	J/molxK	1032.21	Joback Method
cpg	1151.76	J/molxK	1064.76	Joback Method
dvisc	0.0006779	Paxs	485.67	Joback Method

dvisc	0.0003124	Paxs	549.63	Joback Method
dvisc	0.0001692	Paxs	613.60	Joback Method
dvisc	0.0001029	Paxs	677.56	Joback Method
dvisc	0.0000682	Paxs	741.52	Joback Method
dvisc	0.0000482	Paxs	805.49	Joback Method
dvisc	0.0000359	Paxs	869.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U353548&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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